Modeling CO2 plume evolution in oil reservoirs using parallel computing

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Abstract

CO2 sequestration (capture, separation, and long term storage) in various geologic media (such as depleted oil reservoirs, saline aquifers, oceanic sediments) is a possible solution to reduce green house gas emissions. In this study we utilize the PFLOTRAN simulator to investigate geologic sequestration of CO2. PFLOTRAN is a massively parallel 3-D reservoir simulator for modeling subsurface multiphase (CO2, H2O), and multicomponent reactive flow and transport based on continuum scale mass and energy conservation equations. PFLOTRAN has an efficient and modular mechanism to handle variable switching during multiphase transitions, bringing great flexibility in choosing the set of primary variables, addition of new EoS, mixing rules, etc. The multiphase flow equations are sequentially coupled to reactive transport equations describing multi-component chemical reactions within the formation. These reactions consist of aqueous speciation, and precipitation and dissolution of minerals including CO2-bearing phases to describe aqueous and mineral CO2 sequestration. The effect of the injected CO2 on pH, CO2 concentration within the aqueous phase, mineral stability, and other factors can be evaluated with this model. This work is focused on complex density driven flow patterns within both CO2-rich and aqueous phases, and their effect on the long-term containment of injected supercritical CO2. The efficiency of sequestration processes could be affected by many factors, including variations in fluid properties caused by CO2 dissolution and reservoir salinity, changes in geochemical and geophysical properties caused by mineral dissolution and precipitation, etc. This investigation will help provide criteria for site selection and to investigate leakage rates of CO2 to the surface.

PFLOTRAN: Parallel Flow and Reactive Transport

Mathematical Formulation

PFLOTRAN consists of two distinct modules: a mass and energy flow code (PFLOW) and a reactive transport code (PTRAN). The module PFLOW solves mass conservation equations for water and other fluids and an energy balance equation. The module PTRAN solves mass conservation equations for a multicomponent geochemical system. The reactions included in PTRAN involve aqueous species and minerals which can be written in the general form:

$$\sum_i \nu_{ji} A_j \Leftrightarrow A_i \qquad \text{and} \qquad \sum_j \nu_{jm} A_j \Leftrightarrow M_m$$

respectively, where the set of species $\{A_j\}$ refer to a set of primary or basis species in terms of which all other species are written, A_i denotes an aqueous complex referred to as a secondary species, M_m refers to a mineral, and ν_{ji} and ν_{jm} are reaction stoichiometric coefficients derived from an extensive database. The architecture is shown in the right figure.

Mass Conservation: Flow Equations

$$\frac{\partial}{\partial t}\left(\phi s_\alpha \rho_\alpha X_i^\alpha\right) + \nabla \cdot \left[q_\alpha \rho_\alpha X_i^\alpha - \phi s_\alpha D_\alpha^\alpha \rho_\alpha \nabla X_i^\alpha\right] = Q_i^\alpha$$

$$q_\alpha = -\frac{kk_{r\alpha}}{\mu_\alpha}\nabla(p_\alpha - W_\alpha \rho_\alpha gz) \qquad p_\alpha = p_\beta - p_{\alpha\beta}$$

Energy Conservation Equation

$$\frac{\partial}{\partial t}\left[\phi \sum_\alpha s_\alpha \rho_\alpha U_\alpha + (1-\phi)\rho_r c_r T\right] + \nabla \cdot \left[\sum_\alpha q_\alpha \rho_\alpha H_\alpha - \kappa \nabla T\right] = Q_e$$

Multicomponent Reactive Transport Equations

$$\frac{\partial}{\partial t}\left[\phi \sum_\alpha s_\alpha \Psi_j^\alpha\right] + \nabla \cdot \left[\sum_\alpha \Omega_{j\alpha}\right] = -\sum_m \nu_{jm} I_m + Q_j$$

Total Concentration $\Psi_j^\alpha = \delta_{j\alpha} C_j^\alpha + \sum_i \nu_{ji} C_i^\alpha$

Total Solute Flux $\Omega_j^\alpha = (-\tau\phi s_\alpha D_\alpha \nabla + q_\alpha)\Psi_j^\alpha$

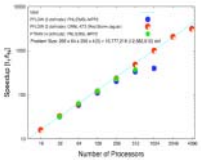
Mineral Mass Transfer Equation

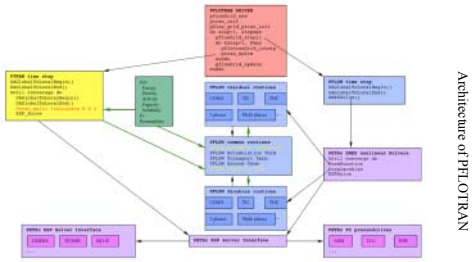
$$\frac{\partial \phi_m}{\partial t} = V_m I_m \qquad \phi + \sum_m \phi_m = 1$$

System closure is accomplished by combining these equations with other auxiliary equations and EoS of phases. Most current EoS, solubility and relative permeability formula were implemented to ensure accuracy, such as Span-Wanger formula for supercritical CO2 phase properties, etc.

Performance and scalability

PFLOTRAN been designed from scratch with parallel scalability in mind, and it displays excellent scaling characteristics on modern supercomputers. The figure at right shows the performance of PFLOW running a one phase thermohydrologic bench mark problem on a 256 x 64 x 256 grid with three degrees of freedom per node (approximately 12.6 million degrees of freedom total). The bench mark was run on both the MPP2 cluster at PNNL/EMSL, a cluster of 1960 1.5 GHz Itanium 2 processors with Quadrics QsNe tII interconnect, and Jaguar, the 5200 Opteron processor Cray XT3 at ORNL/NCCS. PFLOW scales quite well on both machines, bottoming out at around 1024 processors on MPP2, and scaling exceptionally well on Jaguar, displaying linear speedup all the way up to 2048 processors, and still displaying modest speedup when going from there to 4096 processors.





Architecture of PFLOTRAN

Variable switching and phase transition

PFLOW assumes all components exist in system are partly miscible, The solubility is governed by a modified Henry's Law. It employs the commonly used variable switching method to choose certain numbers of primary variables according to Gibbs phase law, resulting in $n_{dof} = n_{comp} + 1$. With this method, the set of primary variables varies for every possible phase combinations in 2^{np}-1 cases, as listed in the table below. Other thermodynamic properties are derived from the primary variables through constraints and equilibrium relations.

Phase transition rules are one of the crucial aspects for implementing the variable switching method. A generic rule to determine if a new phase p forms is that the summation of all mole fractions in the new phase exceeds one, as evaluated from existing phases by pseudo equilibrium, $\sum X_p > 1$; a phase disappears if its saturation is less than zero, $S_p < 0$.

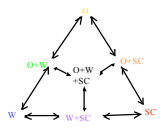
In the numerical implementation, a relaxation method is needed to reduce oscillations and improve performance. Examples below show phase transition diagrams for 3 and 4 phase systems and the selection of primary variables for a 3-phase 3-component system.

Example: 3 components (H2O, CO2, C10H22), 3 phases (Water, Supercritical CO2, oil) system

Primary variable set

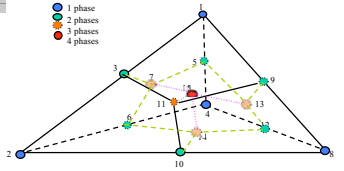
Case	Phase condition	Primary Variables
1	W	P, T, X_W^{CO2}, X_W^{C10}
2	G	P, T, X_W^{CO2}, X_G^{C10}
3	W+G	P, T, S_W, X_G^{CO2}
4	O	P, T, X_W^{CO2}, X_W^{C10}
5	O+W	P, T, S_W, X_W^{CO2}
6	O+G	P, T, S_G, X_G^{CO2}
7	O+W+G	P, T, S_W, S_G

Phase transition diagram



Example: 4 phase system(P1, P2, P3, P4), phase transition diagram

Case	Phase Condition	Case	Phase Condition	Case	Phase Condition
1	P1	6	P2 + P3	11	P1 + P2 +P4
2	P2	7	P1 + P2 + P3	12	P3 + P4
3	P1 + P2	8	P4	13	P1 + P3 + P4
4	P3	9	P1 + P4	14	P2 + P3 + P4
5	P1 + P3	10	P2 + P4	15	P1 + P2 + P3 + P4

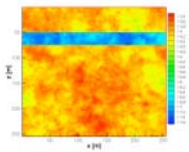


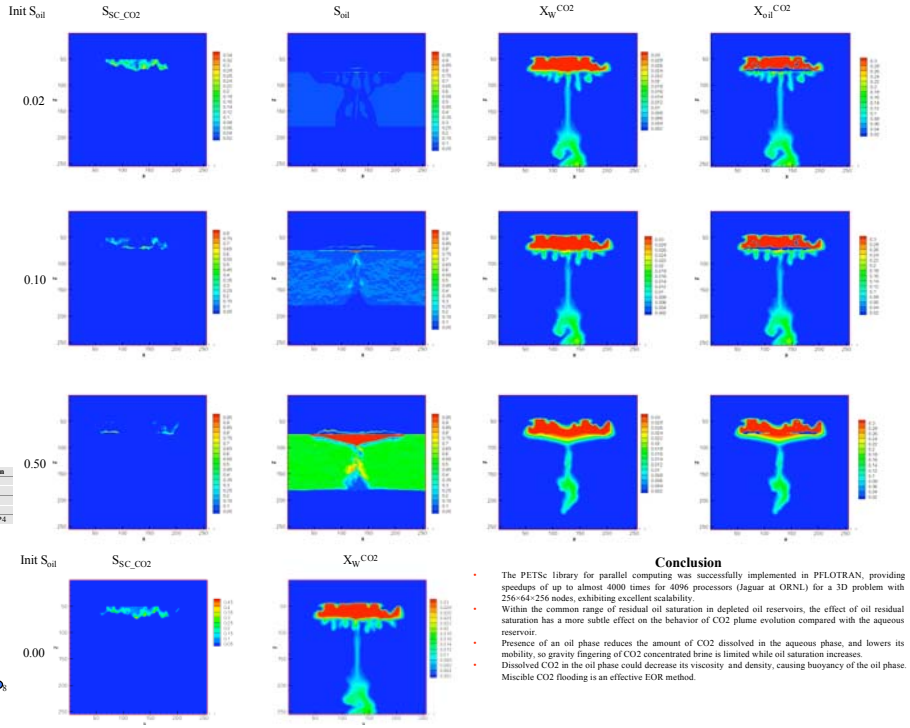
Numerical Simulation

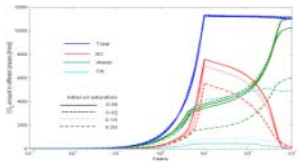
The simulation was conducted for a 2D domain with dimensions 256 x 256m on a uniform grid with 1 x 1m spacing using a random permeability field containing 3 uncorrelated layers with 50m, 25m and 181m thickness, from top to bottom. The log-normal distributed random field is generated by the sequential Gaussian random field generator sgsim from GSLIB, with correlation length 20 m, zero mean and variance 0.25. The values are scaled with the mean permeability of each layer with 10-2, 10-5, 10-2 Darcy, as shown on the right panel. CO2 is injected for 10 years with the rate 1.6x10-4 kg/s at the center of the domain at a depth of 140m.

The initial residual oil is located at depths ranging from 75m to 180m, horizontally across the whole domain. Four cases with different initial oil saturation (0, 0.02, 0.10 ,0.50) are investigated. Outside the dominant oil region, the oil saturation is set to a small value (1x10-4), except for the first case, in which the oil residual is zero everywhere.The relative permeability is determined by linear interpolation. No capillary effect is considered.

Snapshots of saturation and concentration at 400 years are shown in the right panel.







Distribution of CO2 in phases

Conclusion

- The PETSc library for parallel computing was successfully implemented in PFLOTRAN, providing speedups of up to almost 4000 times for 4096 processors (Jaguar at ORNL) for a 3D problem with 256×64×256 nodes, exhibiting excellent scalability.
- Within the common range of residual oil saturation in depleted oil reservoirs, the effect of oil residual saturation has a more subtle effect on the behavior of CO2 plume evolution compared with the aqueous reservoir.
- Presence of an oil phase reduces the amount of CO2 dissolved in the aqueous phase, and lowers its mobility, so gravity fingering of CO2 concentrated brine is limited while oil saturation increases.
- Dissolved CO2 in the oil phase could decrease its viscosity and density, causing buoyancy of the oil phase. Miscible CO2 flooding is an effective EOR method.

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References

Balay, S., Gropp, W.D., McInnes, L.C. and Smith, B.F., "Efficient Management of Parallelism in Object Oriented Numerical Software Libraries", *Modern Software Tools in Scientific Computing*, Ed. Arge, E., Bruaset, A. M. and Langtangen, H. P., 163–202, Birkhauser Press. (1997)